

6-Chloro-N²-ethyl-N⁴-propyl-1,3,5-triazine-2,4-diamine
90952-64-0 | DTXSID60536638

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.43

Global applicability domain: Inside

Local applicability domain index: 5.79e-01

Confidence level: 8.91e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Atrazine</div> <div>Measured: 2.61</div> <div>Predicted: 2.67</div>	<div>Image not found</div> <div>Simazine</div> <div>Measured: 2.18</div> <div>Predicted: 1.97</div>
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